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Local Structure Preserving Algorithms for Molecular Beam Epitaxial Models with Slope Selection Based on Energy Quadratization Method

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Abstract. A molecular beam epitaxial (MBE) model with slope selection consisting of a fourth order Ginzburg-Landau double well potential, is derived from the variation of the free energy. One challenge in constructing the local structure preserving algorithms (SPAs) for the MBE model with slope selection is how to properly discretize the equation in space and time simultaneously in order to preserve the local structure at the discrete level. To resolve this issue, we employ the local energy dissipation property and the energy quadratization techniques. One novelty is that all nonlinear terms are treated semi-explicitly. The other novelty is that we introduce proper intermediate variables to make the space operators act on one single term, which is one crucial step in constructing local SPAs. We then develop two local energy dissipation preserving schemes and show rigorously the local energy dissipation property of the two schemes. Under suitable boundary conditions, such as periodic boundary conditions, the algorithms can preserve not only mass but also global energy dissipation property. Numerical experiments confirm the second-order accuracy and show the excellent performance of the schemes proposed.

AMS subject classifications: 65M06, 80M20

Key words: Molecular beam epitaxial model, energy quadratization method, linear, finite difference, local structure preserving.

1. Introduction

The molecular beam epitaxy is a popular technique widely used for growth of single-crystal thin films, quantum wells, superlattices, and similar structures. It was developed

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first as a research system for preparing single-crystal thin films and superlattices [22]. Nowadays it is used in many fields, including the production of electronic goods, optimal devices, and sensors. It has a wide range of applications in digital economy, energy, and semi-conductor nanotechnology [28]. The model is a gradient flow derived from the variation of a given effective free energy. It is based on the generalized Onsager principle [8], which ensures the energy dissipation of the gradient flow both locally and globally. This motivates us to develop numerical simulation tools to inherit this property.

There is a variety of numerical solvers having the global energy dissipation property of the gradient flow at the discrete level. They are called the energy stable schemes. Let us briefly recall well-known techniques used in this field. We first introduce a convex-splitting method. It is proposed in [9] and its main idea consists in splitting the free energy density into concave and convex terms in order to ensure the system energy dissipation. Chen *et al.* [5] applied this technique to the molecular beam epitaxy model without slope selection, while Wang *et al.* [23] used it when considering the modified phase field crystal equation. For more information about this approach the reader can consult Refs. [11, 25]. Christlieb *et al.* [7] proposed an implicit nonlinear scheme and noted that the splitting error of convex splitting methods might lead to misleading results. Chen *et al.* [4] developed a stabilized decoupled time discretization scheme for coupled nonlinear systems of classical phase-field vesicle membrane models. Using stabilization method, Shen *et al.* [21] developed a number of commonly used numerical schemes for the Allen-Cahn and Cahn-Hilliard equations. In order to preserve the energy dissipation rate, an auxiliary variable turning the free energy density into a quadratic term has been used. It was first introduced in [12] to deal with the Cahn-Hilliard and Allen-Cahn equations and termed energy quadratization (EQ) method. Later on, Yang *et al.* [27] used the above approach to develop unconditionally energy stable schemes for the viscous Cahn-Hilliard equation with hyperbolic relaxation. They treated all nonlinear terms semi-explicitly. However, since the EQ method is not applicable to all systems, the scalar auxiliary variable (SAV) method has been developed. Shen *et al.* [19,20] applied the SAV method to a large class of gradient flows and studied its convergence and errors for L^2- and H^{-1}-flows with a typical form of the free energy. New methods for gradient flow models — viz. projection and the Lagrange multiplier or the supplementary variable method have been studied recently [6, 13, 17]. This approach can also preserve the global energy dissipation law and capture the dynamics.

Up to now, much efforts have been spent to develop numerical schemes for the MBE model [5,26], where main challenge consists in the discretization of nonlinear terms while preserving the energy dissipation law. Yang *et al.* [28] applied the EQ method to the MBE model with the main idea of transforming the free energy into a quadratic function and treating nonlinear terms semi-explicitly to obtain a semi-discrete linear system at each time step. Motivated by this idea, we aim to develop local SPAs for the MBE model with slope selection which has been applied with EQ method. Lu *et al.* [15] considered local SPAs for the MBE model and presented an MBE model with slope selection, which has the local energy dissipation property at continuous and discrete levels. Actually, the local SPAs have advantages over global SPAs because they do not rely on boundary conditions. Moreover, with suitable boundary conditions — e.g. periodic ones, local SPAs can preserve the global